PG Diploma in Cheminformatics

Syllabus

UNIVERSITY DEPARTMENT

Program Code: ****

2021 – 2022 onwards

BHARATHIAR UNIVERSITY

(A State University, Accredited with "A" Grade by NAAC,
Ranked 13th among Indian Universities by MHRD-NIRF,
World Ranking : Times - 801-1000, Shanghai - 901-1000, URAP – 1047)

Coimbatore - 641 046, Tamil Nadu, India

Program Educational Objectives (PEOs)	
The **PG Diploma in Cheminformatics** program describe accomplishments that graduates are expected to attain within five to seven years after graduation	
PEO1	Should be aware of available Cheminformatics resources and information in databases
PEO2	Apply critical, analytical and problem solving skills to deal with Cheminformatics research
PEO3	Gain a deep understanding of the biomolecular systems
PEO4	Attain knowledge to identify the research problems in Cheminformatics
PEO5	Develop very efficient algorithms to extract biological knowledge from complex dataset
PEO6	Develop programming skills to write their own codes and scripts to resolve research accomplishments
PEO7	Possess drafting and writing skills to enhance scientific communication
PEO8	Update in accordance with recent scientific advancements and technology
PEO9	Gain higher level degrees to pursue a career in academics or scientific organizations
PEO10	Should be able to pursue research and also in industry placement in the sectors of pharmaceutical, agricultural, environmental science and food industries

Program Specific Outcomes (PSOs)	
After the successful completion of PG Diploma in Cheminformatics program, the students are expected to	
PSO1	Develop applications to solve biological problems by utilizing the Cheminformatics algorithms and programming languages
PSO2	Manipulate scientific datasets and retrieve and access them through biological databases
PSO3	Develop knowledge and skills to analyses and interpret biological data for research requirements
PSO4	Develop good scientific communication skills
PSO5	Gain knowledge of the tools, frameworks, and libraries for Cheminformatics applications
PSO6	Undergo seminars, conferences and hands on workshops to facilitate domain expertise

Program Outcomes (POs)	
On successful completion of the M. Sc. Bioinformatics program	
PO1	Should be able to understand the basic principles and concepts of biology, chemistry, computer science and mathematics
PO2	Able to apply the knowledge in Cheminformatics such as computational biology, chemical principles that underlie biochemistry, molecular biology and genomics
PO3	Develop and implement software effectively to retrieve information from biological databases and use this information for computation
PO4	Comprehend and provide solution to enable designing and implementing new algorithms and analysis methods
PO5	Understand the concept of intersection of life and information sciences, structure-function relationships, information theory, gene expression, and database queries
PO6	Develop computational techniques and diversified bioinformatics tools for processing data, including statistical, machine learning and data mining techniques
PO7	Design and implement efficient and reliable Cheminformatics solutions by optimizing the usage of existing tools and developing new ones
PO8	Analyze and think critically the research methods in Cheminformatics such as dissertation, research, preparation and presentations at scientific meetings, seminars and qualifying examinations
PO9	Develop an insight into scientific methodology and advances in Cheminformatics research
PO10	Have an understanding of current technology trends as well as future directions and recognize the need and develop the skills necessary for professional development

BHARATHIAR UNIVERSITY: COIMBATORE 641 046

PG Diploma in Cheminformatics

Curriculum (University Department)

(For the students admitted during the academic year 2021 – 22 onwards)

Course Code	Title of the Course	Credits	Hours		Maximum Marks		
			Theory	Practical	CIA	ESE	Total
FIRST SEMESTER							
13A	Basics of Cheminformatics	5	60	-	50	50	100
13B	Computer Programming for Cheminformatics	5	60	-	50	50	100
13C	Cheminformatics Database Design and Their Management	5	60	-	50	50	100
13D	Pharmaceutical Chemistry	5	60	-	50	50	100
Total		**20**	-	-	**200**	**200**	**400**
SECOND SEMESTER							
23A	Structure Based Drug Design	5	60		50	50	100
23P	Practical-I: Computer Programming	5	-	60	50	50	100
23Q	Practical – II: Computer Aided Drug Design	5	-	60	50	50	100
27V	Project & Viva-Voce	10	-	-	50	50	100
Total		**25**			**200**	**200**	**400**
Grand Total		**45**	-		**400**	**400**	**800**

First Semester

Course code	13A	BASICS OF CHEMINFORMATICS	L	T	P	C
Core/Elective/Supportive		Core	5	-	-	5
Pre-requisite		Basic Knowledge in Chemistry	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. Explain the primary and secondary structures of proteins with stereochemistry.
2. Retrieve chemical information from structural and visualization tools.
3. To make students familiar on existing databases and their application.
4. Give a clear view on algorithms which is involved in biomolecular networks.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Understand the mathematical implementation in molecular networks.	K1
2	Evaluate the importance of protein structure in drug designing.	K2
3	Describe chemical data retrieval from the databases.	K3
4	Know the various tools in proteomics, genomics and metabolomics.	K4
5	Structure based designing of ligand with a help of QSAR.	K5

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** - Create

Unit:1	Molecular Numerology	12 hours

Graph theory and molecular numerology; Logic, sets and functions; Algorithms, integers and matrices; Mathematical reasoning, induction and recursion; Counting; graphs, trees and sets, basic probability and statistics; Markov processes. Application: Biomolecule Networks, Metabolic Pathways.

Unit:2	Stereochemistry	12 hours

Basic Stereochemistry, Amino acids and Proteins and Properties; pKa, pH and ionization of acids and bases; Protein structure - Primary structure, Secondary structure - helix & sheet; Tertiary structure; Quaternary structure; covalent and non-covalent forces that maintain structures. Introduction to drug action, pro drug design and applications.

Unit:3	Chemical Information	12 hours

History of scientific information communication-chemical literature-chemical information-chemical information search-chemical information sources-chemical name and formula searching-analytical chemistry-chemical history-biography-directories and industry sources. Chemical Structure: Databases, Formats, Drawing Tools and Structure Visualizations.

Unit:4	Database Management	12 hours

Introduction to data and Database; Data Type; Experimental sources of biological data; Publicly available databases; Database Management; Gene expression monitoring; Genomics and Proteomics; Metabolomics; Visualization of sequence data; Visualization of structures using Rasmol or Pymol or CHIME; Genetic basis of disease; Personalised medicine and gene-based diagnostics.

Unit:5	Structure-Based Drug Design	12 hours

Introduction to drugs, Chemical structural databases, Structure-based drug design, Protein

structure, Drug action & enzymes. Drug action & receptors, Drug Design, Ligand-Based Design and *De Novo* Drug Design Virtual screening/docking of ligands. Pharmacophore Design, Molecular similarity and molecular descriptors. Prediction of Binding Modes, Protein–Ligand binding free energies, ADMET prediction, QSAR and 3D-QSAR Methods.

	Total Lecture hours	**60 hours**

Reference Books

1	"Mathematical Methods for Physicists" Arfken, Academic Press 1985
2	Schaum's Outline of Probability and Statistics, Murray R Spiegel, John J. Schiller, R. Alu Srinivasan
3	Stereochemistry, by David G. Morris, Eddie Abel
4	Introduction to Protein Structure: Second Edition, Carl Branden , John Tooze
5	Combinatorial Chemistry and Molecular Diversity in Drug Discovery, Eric M. Gordon, James F. Kerwin
6	Computer-Aided Drug Design: Methods and Applications, T.J. Perun C.L. Propst
7	Chemical Information Sources (Mcgraw-Hill Series in Advanced Chemistry) ,Gary Wiggins
8	Introduction to Bioinformatics, Teresa K. Attwood, David Parry-Smith
9	Molecular Modeling: Basic Principles and Applications, 3rd Edition,Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers
10	Trends in Bioinformatics. By Dr. P. Shanmughavel. 2006 Pointer publishers, Jaipur, India.
11	Principles of Bioinformatics. By Dr. P. Shanmughavel. 2005 Pointer publishers, Jaipur, India.

Course Designed By: Dr.P.Shanmughavel & Dr.V.Hemamalini

Mapping with Programme Outcomes

COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO 10**
CO1	S	S	S	S	M	S	M	S	S	M
CO3	M	M	M	S	S	M	S	M	M	M
CO3	S	M	S	S	M	S	M	S	S	S
CO4	M	S	M	S	S	S	S	M	S	S
CO5	S	M	M	M	M	M	S	S	M	S

*S-Strong; M-Medium; L-Low

Course code	13B	COMPUTER PROGRAMMING FOR CHEMINFORMATICS	L	T	P	C
Core/Elective/Supportive		Core	5	-	-	5
Pre-requisite		Basic Knowledge in Programming	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. To understand the Languages and programmes in operating system.
2. Familiarize the students in programming languages and their applications.
3. To keep the students update in various up comings like machine learning.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Understand various terminologies in computer languages.	K1
2	Have a good understanding in the concepts of C & C++.	K2
3	Objective oriented JAVA programming in cheminformatics.	K2
4	Be able to perform programming in PERL & PYTHON.	K6
5	Create awareness and familiar on Machine Learning.	K6

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** - Create

Unit:1	Operating System	12 hours

Operating systems – Human interface, Algorithms-genetic algorithms- neural networks- Artificial intelligence, Grid & high-performance computing, Software, Open source. Document markup languages: HTML, XHTML, XML: Key terminology, Characters and escaping, Well-formedness and error-handling, Schemas and validation Related specifications, Use on the Internet, Programming interfaces, Chemical Markup Language.

Unit:2	Basics of C & C++	12 hours

Basics of C & C++ : Basic Syntax - Variables, Constants and Built-in Types - Operators and Basic Expressions - Flow Control and Statement Blocks - Functions and Arguments - Modules and Scope – Arrays - Character Strings – Pointers - Defining New Types - Classes and Objects – Casts – Preprocessor The Programming Process - Writing Source Code.

Unit:3	JAVA Programming	12 hours

JAVA Programming -Introduction to Java - JavaScript for Cheminformatics: Basic Syntax - Variables, Constants and Built-in Types - Operators and Basic Expressions - Flow Control and Statement Blocks - Functions and Arguments - Modules and Scope – Arrays - Character Strings – Pointers - Defining New Types - Classes and Objects – Casts – Preprocessor

Unit:4	Programming in PERL and PYTHON	12 hours

Programming in PERL and PYTHON: PERL: Introduction, Basic operators and control structures, Scalars, Lists, Hashes, File Manipulation, Pattern Matching and Regular Expressions, Subroutines, Text and string Processing Python Programming: Overview-Data structures-control flow-modules-basic I/O, Exception Handling, Regular expressions, File manipulation, classes, standard library.

Unit:5	Machine Learning	12 hours
Machine Learning: Definition of learning. Representation and prior knowledge. Neural Networks, Supervised, Unsupervised, and Semi-Supervised Learning, Deep Learning and Linear Regression. Algorithms and Model Selection: Linear Regression, Linear Regression Assessment, Logistic Regression, Naive Bayes; Evaluating and choosing the best hypothesis; Model selection.		
	Total Lecture hours	**60 hours**

Reference Books

1	Introduction to Machine Learning. E.Alpaydin, 3rd Edition, 2014, MIT Press.
2	The Machine Learning Approach – P.Baldi, S.Brunak, F.Batch - 2014, MIT Press.
3	Programming Perl - Tom Christiansen, Larry. Wall Orielly Publications
4	The C Programming Language, B.W.Kernighan and D.M. Ritchie 2nd Edition. Prientice Hall of India.
5	Programming Perl – Larry Wall, Tom Christiansen & John Orwant 3ed 2000- O' Reilly.
6	Programming Python – Mark Lutz – 2nd Ed., O' Reilly
7	E. Balagurusamy - "Programming in C++ " - Tata Mc. Graw Hill Edition
8	Byron Gottfried, - "Programming with C" (Schaum's Outline Series) - Tata
9	McGrawHill Publishing Company - 1998.
10	Object oriented programming with c++ -Robert Laffore -Waite series.

Course Designed By: Dr.N.Jeyakumar & Dr.P.Shanmughavel

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	M	S	S	S	M	S	M	S	M	M
CO2	S	M	S	M	S	M	S	M	S	M
CO3	M	S	M	S	M	S	M	S	S	S
CO4	S	S	S	M	S	M	S	M	M	S
CO5	S	M	M	M	M	S	S	M	S	M

*S-Strong; M-Medium; L-Low

Course code	13C	CHEMINFORMATICS DATABASE DESIGN AND THEIR MANAGEMENT	L	T	P	C
Core/Elective/Supportive		Core	5	-	-	5
Pre-requisite		Basic Programming and Database Knowledge	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. Give a clear view on databases and their basic concepts.
2. To make the students capable using data mining methods.
3. Understand the availability of chemical databases.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Have a good understanding of databases and its recovery.	K2
2	Evaluate network and hierarchial data models.	K2
3	Remember the dependencies of Schema refinement	K1
4	Explain all the features of chemical databases.	K4
5	Apply data mining methods in human genome.	K3

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** - Create

Unit:1	Database Concepts	12 hours

Database Concepts: Relational Databases-Object Databases-Basic SQL- Data types- Operators. E-R Model and Normalization - Entity and entity sets; Relations and relationship sets; E-R diagrams; Reducing E-R Diagrams to tables; Security, Backup and Recovery: Creating users- Encrypting traffic- Backup of the database- Recovery

Unit:2	Network Data Model	12 hours

Network Data Model: Basic concepts; Hierarchical Data Model: Basic Concepts; Multimedia Databases - Basic Concepts and Applications; Indexing and Hashing; Text Databases; Introduction to Distributed Database Processing, Data Security. Interfacing programs with databases; Data interoperability using XML.

Unit:3	Database Design	12 hours

Database Design: Introduction to Schema Refinement- Functional Dependencies-Normal Forms- First, Second, Third, Boyce code, Fourth and Fifth Normal forms- Multivalued Dependencies.

Unit:4	Chemical Databases	12 hours

Introduction- chemical databases - types- chemical database design - Bio Catalysis Database. The MOS Database, reaction databases, The Failed Reaction Database. Protecting groups database-solid-phase synthesis database- Sequence Databases, Spectra. Databases, (Bio) Activity/Prop. Databases, Toxicology Databases.

Unit:5	Data Mining Methods	12 hours

Data mining methods, Sub structural analysis, Discriminant Analysis, Neural networks, Decision Trees; Software for Chemical Data Mining. Data Mining and human genome. Combinatorial Chemistry Technologies and Libraries. Chemistry Libraries: Design of Focused, Diverse and

Thematic Libraries. Biological Libraries, Bio planning, Peptide Display Libraries design and construction.

	Total Lecture hours	**60 hours**

Text Book(s)

1	Practicals in Bioinformatics By Dr. P. Shanmughavel and Gulshan Wadhwa, 2010 Pointer publishers, Jaipur, India.
2	Database Systems Concepts ,Abraham Silberschatz, Henry F. Korth, S. Sudarshan
3	Database Management Systems, Raghu Ramakrishnan, Johannes Gehrke
4	Data Mining Techniques,Michael Berry & Gordon Linoff

Course Designed By: Dr.S.Usha & Dr.C.Jayaprakash

Mapping with Programme Outcomes

COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	S	S	S	S	M	S	M	S	S	M
CO3	S	M	S	M	S	M	S	M	S	S
CO3	M	S	S	S	S	S	M	S	M	M
CO4	S	S	S	M	S	M	S	M	S	S
CO5	S	M	S	M	S	M	S	M	S	M

*S-Strong; M-Medium; L-Low

Course code	13D	PHARMACEUTICAL CHEMISTRY	L	T	P	C
Core/Elective/Supportive		Core	5	-	-	5
Pre-requisite		Basic Chemistry and Knowledge in Pharma	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. Make the students understand the necessity of modeling in drug discovery.
2. To use the available databases to get 3D structures.
3. Provide an understanding on Combinatorial Library Design Strategies.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Understand the patent and patent databases.	K2
2	To apply biological and structural data in designing.	K3
3	Describe similarity methods and clustering analysis.	K3
4	Know the 3D Databases in Experimental and Theoretical way.	K4
5	conduct experiments Chemical Reactions, Reaction Prediction and Synthesis Design	K5

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** - Create

Unit:1	Structure Representation	12 hours

Representation of 2D & 3 D Molecular Structures - Computer Representations, Graph Theoretic Representations, Connection Tables and Linear Notations, Canonical Representations. Chemical Databases, Reaction databases, Representation of patents and patent databases. Structure and sub-structure search.

Unit:2	Molecular Descriptors & QSAR	12 hours

Structural data, Biological data - Molecular Descriptors - Descriptors Calculated from the 2D Structure, Descriptors Calculated from the 3D Representations, Data verification and manipulation. Deriving a QSAR Equation - Simple and Multiple Linear Regression, Designing a QSAR "Experiment", 3D-QSAR, Nonlinear Models, Model validation, Principal Components Regression, Partial Least Squares, Molecular Field Analysis and Partial Least Squares.

Unit:3	Similarity Methods	12 hours

Similarity Methods - Similarity Based on 2D Fingerprints, Similarity Coefficients, 2D Descriptor Methods, 3D Similarity Methods. Selecting diverse Sets of Compounds - Cluster Analysis, Dissimilarity-Based Selection Methods, Cell-Based Methods, Optimization Methods.

Unit:4	Pharmacophore Modeling	12 hours

3D Databases – Experimental and Theoretical, 3D Pharmacophores, Methods to derive 3D Pharmacophore, Pharmacophore Model validation, 3D Pharmacophore Mapping and 3D Database Searching.

Unit:5	Combinatorial Chemistry and Library Design	12 hours

Combinatorial Chemistry and Library Design - Diverse and Focused Libraries, Library Enumeration, Combinatorial Library Design Strategies, Approaches to Product-Based Library Design,

Multiobjective Library Design, Practical Examples of Library Design, High throughput screening (HTS). Chemical Reactions, Reaction Prediction and Synthesis Design.

	Total Lecture hours	**60 hours**

Reference Books

1 An Introduction to Chemoinformatics by Andrew R. Leach and Valerie J. Gillet. Springer Publisher

2 Applied Chemoinformatics - Achievements and Future Opportunities. Edited by Thomas Engel and Johann Gasteiger. Wiley-VCH publisher.

Course Designed By: Dr.S.Usha

Mapping with Programme Outcomes

COs	**PO1**	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PO7**	**PO8**	**PO9**	**PO10**
CO1	S	S	S	S	M	S	M	S	S	M
CO3	S	M	M	M	S	M	S	M	S	S
CO3	S	S	S	S	S	S	S	S	S	M
CO4	S	S	S	S	S	S	S	M	M	S
CO5	S	M	M	M	M	M	S	M	M	M

*S-Strong; M-Medium; L-Low

Second Semester

Course code	23A	STRUCTURE BASED DRUG DESIGN	L	T	P	C
Core/Elective/Supportive		Core	5	-	-	5
Pre-requisite		Basic Knowledge in Bioinformatics	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. Provide the detailed note on the strategies of Drug discovery and drug activity.
2. To describe how to use algorithms, to rectify our quarries.
3. Implementation of various approaches in ligand designing.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	To use various strategies for the activity and discovery of drugs.	K3
2	Understand the concepts of molecular dynamics.	K2
3	Analyze potential approach of QSAR in Molecular field analysis.	K3
4	Apply De novo drug design approach in ligand prediction.	K4
5	Evaluate Deep learning, feature and similarity based approaches in molecular docking.	K5

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** - Create

Unit:1	Drug Discovery	12 hours

Drug discovery-Strategies and historical developments - Introduction –conventional strategies to drug discovery-molecular mimetic- first and second generation rational approach-Rational drug design-assessment of drug activity.

Unit:2	Molecular Dynamics	12 hours

Introduction, Molecular Dynamics using simple models. Dynamics with continuous potentials. Constant temperature and constant dynamics. Conformation searching, Systematic search. Applications to protein folding.

Unit:3	QSAR Approach	12 hours

Developing and using QSAR- QSAR-validation methods-3D QSAR approach-QSAR descriptors, 3D QSAR-Introduction-Pharmacophore identification-binding site modeling of unknown receptor-receptor mapping-structural alignment and superposition-molecular field analysis (MFA).

Unit:4	De Novo Drug Design	12 hours

3D pharmacophore, De novo Ligand design-introduction-approaches to de novo drug design problem-some current methods for de novo design.3D data base searching and virtual screening, Sources of data, molecular similarity and similarity searching, prediction of binding energy of ligand-receptor complex-Free energies and salvation-electrostatic and non-electrostatic contribution

Unit:5	Molecular Docking	12 hours

Molecular docking: Introduction to docking approaches: Rigid docking, Flexible docking - Shape complementarily- Simulation Mechanics of docking - Search Algorithm-Scoring Function-Applications. Machine Learning applications in virtual screening: Similarity based approach,

Feature based approach, Deep Learning Approach.		
	Total Lecture hours	**60 hours**

Reference Books

1	The organic chemistry of drug design and drug action, Richard B. Silverman
2	Drug design: cutting edge approaches, Darren R. Flower
3	Molecular Modeling: Basic Principles and Applications, 3rd Edition, Hans-Dieter Höltje, Wolfgang Sippl, Didier Rognan, Gerd Folkers
4	Molecular Modelling: Principles and Applications, Andrew R. Leach
5	Trends in Bioinformatics. By Dr. P. Shanmughavel. 2006 Pointer publishers, Jaipur, India.
6	Principles of Bioinformatics. By Dr. P. Shanmughavel. 2005 Pointer publishers, Jaipur, India.
7	Deep Learning for the Life Sciences: Applying Deep Learning to Genomics, Drug Discovery – Bharath Ramsundar,2019 – O'Reilly Publishers

Course Designed By: Dr.P.Shanmughavel & Dr.S.Usha

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	M	S	M	S	S	S	S	S	M	M
CO3	S	M	M	M	S	M	S	M	S	S
CO3	M	M	S	S	S	S	M	S	S	M
CO4	S	S	S	S	M	S	S	M	M	S
CO5	S	M	M	S	M	S	M	M	S	M

*S-Strong; M-Medium; L-Low

Course code	23P	PRACTICAL-I: COMPUTER PROGRAMMING	L	T	P	C
Core/Elective/Supportive		Core	-	-	5	5
Pre-requisite		Basic Knowledge in Programming	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. To understand the computational languages and programs.
2. To know the application of computer programming.
3. To make students understand various coding languages and their intensity.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	To make remember the features of programs.	K1
2	Understand the object-oriented programming language.	K2
3	To learn about text manipulation and apply for a wide range of tasks.	K3
4	Create a support on modules and packages, which encourages program modularity and code resuse.	K6

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

1.	**C++** - Class, Functions and Object oriented programming	
2.	**JAVA** - Class, Objects and Inheritance	
3.	**Perl** - Loop, Subroutine and File Handling	
4.	**Python** - Loop, Functions, Classes and Objects	
5.	**Visual Basic** - Classes & Objects, Basic Controls, File Handling and Dialog Boxes	
6.	**MySQL –** SQL operations, Database Connectivity and Producing Reports	

Total Lecture hours	**60 hours**

Designed By: Dr.N.Jeyakumar & Dr.P.Shanmughavel

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	M	S	S	S	S	S	S	S	S	S
CO2	S	S	S	M	S	S	M	S	M	M
CO3	S	M	S	S	M	M	S	M	S	S
CO4	M	S	S	S	S	S	S	S	S	S

*S-Strong; M-Medium; L-Low

Course code	23Q	PRACTICAL – II: COMPUTER AIDED DRUG DESIGN	L	T	P	C
Core/Elective/Supportive		Core	-	-	5	5
Pre-requisite		Basic Knowledge in Bioinformatics	Syllabus Version		2021-22	

Course Objectives:

The main objectives of this course are to:

1. To Understand various types of databases and their utility to solve various quarries.
2. To learn how to build new chemical structures.
3. To understand how to derive, represent and manipulate the structures and reactions of molecules.

Expected Course Outcomes:

On the successful completion of the course, student will be able to:

1	Analyze computational modeling methods to reveal the relationships between structural properties of chemical compounds.	K2
2	To understand the spatial structures of molecules in different states like gaseous, liquid and solid.	K2
3	To evaluate how two or more molecular structures fit together	K5
4	Analyzing the physical movements of atoms and molecules.	K6

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

1	**Chemical databases –** ChemBank - ChemBioFinder – CSChemoffice - ZINC	
2	**Small Molecule Building –** Chemsketch, ISIS Draw	
3	**Molecular Modeling –** Modeller, Swisspdb	
4	**Molecular dynamics -** GROMACS- NAMD-VEGA ZZ	
5	**Structural chemistry -** NWChem –GAMESS	
6	**Docking -** Auto dock, DOCK -VEGA- FlexX	
7	**ADME Prediction –** SwissADME, PreADMET	
8	**Toxicity Prediction -** Toxinpred, ProTox -II	
9	**QSAR Prediction**	
	Total Lecture hours	**60 hours**

Reference Books

1 Practicals in Bioinformatics By Dr. P. Shanmughavel and Gulshan Wadhwa, 2010 Pointer publishers, Jaipur, India.

Course Designed By: Dr.S.Usha & Dr.C.Jayaprakash

Mapping with Programme Outcomes

COs	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	S	S	S	S	S	S	S	M	S	S
CO2	S	M	S	M	S	S	M	S	M	S
CO3	M	S	S	S	M	M	S	M	S	S
CO4	S	S	S	S	S	S	S	S	S	S

*S-Strong; M-Medium; L-Low